

The Crystal Structure Of Thymoquinone

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Beamline(s): X3B1

Introduction: Thymoquinone is an organic compound found in black cumin (*Nigella Sativa* Linn), with pharmaceutical uses in the treatment of asthma and arthritis. The molecule ($C_{10}O_2H_{12}$) is shown in figure 1 and it has one internal degree of freedom.

Methods and Materials: The high resolution X-ray powder diffraction data has been taken at the beamline X3B1. The diffraction pattern has been indexed using the program TREOR. The triclinic cell (after Rietveld refinement) is $a=6.73922(3)$ Å, $b=6.93129(3)$ Å, $c=10.50103(5)$ Å, $\alpha=91.4076(8)^\circ$, $\beta=97.5659(5)^\circ$, $\gamma=77.1445(4)^\circ$, Cell volume = $474.054(4)$ Å³. The estimation of density suggested $Z=2$.

A Le Bail fit was done using the program GSAS (Rwp=7.23%). For the structure solution, $Z=2$ in both possible space groups $P\bar{1}$ and $P1$ were tried. This implies 7 or 14 structural parameters respectively.

The molecular geometries of several fragments containing the quinone ring were downloaded from Cambridge Structural Database. The complete molecular structure was built with the program Chem3D. The crystal structure was solved with the program PSSP [1] using the first 47 integrated intensities.

Results: Solutions with very similar agreement factors were obtained in both space groups ($S=0.15$). After the Rietveld refinement the inversion symmetry was corroborated. The Rietveld refinements were done with the program GSAS, Rwp=10.66%. In figure 2 is represented the crystal structure obtained. The Rietveld plot is shown in figure 3.

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References: [1]. Program PSSP. Available at <http://powder.physics.sunysb.edu>.

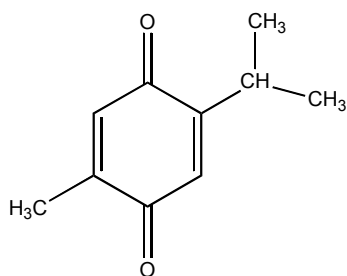


Figure 1: The molecule of Thymoquinone

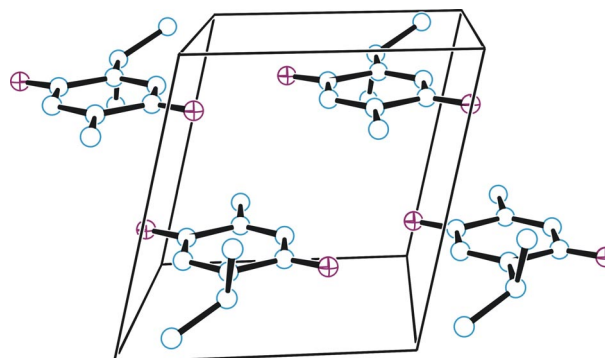


Figure 2: The crystal structure of Thymoquinone. Hydrogen positions were not determined.

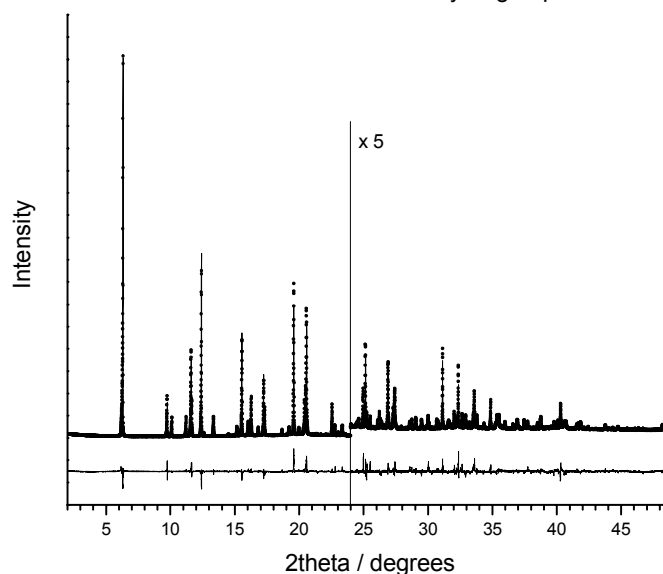


Figure 3: Plot of the Rietveld refinement.